

Intermediate-Level Crossings of a First-Passage Path

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Abstract.

We investigate some simple and surprising properties of a one-dimensional Brownian trajectory with diffusion coefficient D that starts at the origin and reaches X either: (i) at time T or (ii) for the first time at time T . We determine the most likely location of the first-passage trajectory from $(0, 0)$ to (X, T) and its distribution at any intermediate time $t < T$. A first-passage path typically starts out by being repelled from its final location when $X^2/DT \ll 1$. We also determine the distribution of times when the trajectory first crosses and last crosses an arbitrary intermediate position $x < X$. The distribution of first-crossing times may be unimodal or bimodal, depending on whether $X^2/DT \ll 1$ or $X^2/DT \gg 1$. The form of the first-crossing probability in the bimodal regime is qualitatively similar to, but more singular than, the well-known arcsine law.

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1. Introduction

While Brownian motion has been extensively studied and much is well understood about this process (see, e.g., [1–4]), a number of simple questions continue to be investigated when the motion is subject to a constraint. Some examples of this genre include determining the time that Brownian path spends in a range dx about a point x [5–7], the area swept out by a Brownian motion when it first returns to the origin [8–11], the time when a one-dimensional Brownian motion, which starts at $x > 0$, attains its maximum before first crossing the origin [12, 13], as well as related extremal properties of such motions [14]. There has also been considerable study on the topic of level-crossings, namely, the crossings of a given point on the line, for both Brownian motion [15, 16] and for general stochastic processes [17–19], as well as investigations of the crossings of a time-dependent level (see, e.g., [2, 15, 20–24]).

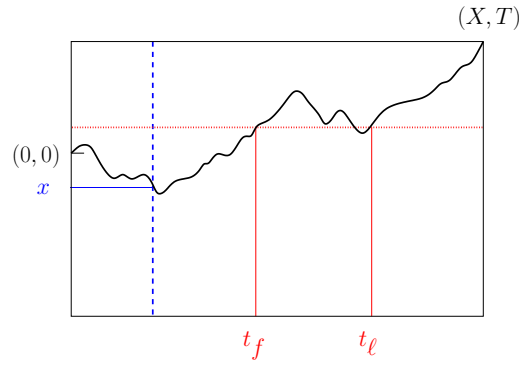


Figure 1. Illustration of the quantities under study. Shown is a schematic first-passage path from $(0,0)$ to (X,T) . At some intermediate time (dashed line), the particle is at position x . At some intermediate level (dotted line), the first- and last-crossing times of this level are t_f and t_l .

Given these extensive studies, it is surprising that some basic issues about level crossings seem to have not yet been fully addressed. In this work, we investigate the intermediate-level crossings in both space and time of a Brownian motion that *first* reaches a final destination $X > 0$ at time T . This type of question underlies the task of reconstructing a Brownian path from measurements at discrete times, an issue that is of basic importance for understanding diffusion in porous media (see, e.g., [25–27]). The condition that the particle must reach X for the first time at time T constrains the entire trajectory before time T in a non-trivial way. We will study the consequences of this constraint on the following basic properties of a Brownian particle with diffusivity D at intermediate stages on its way to its first passage at (X,T) , as illustrated in Fig. 1:

- (i) At an arbitrary intermediate time, what is the expected position x of the particle?
- (ii) When does the particle *first* cross an intermediate level $x < X$?
- (iii) When does the particle *last* cross this intermediate level?

Our approach to answer these questions is based on decomposing the first-passage probability to (X, T) as the convolution of the propagator to the intermediate point (x, t) and the propagator from this intermediate to the final point. In this framework, the intermediate crossing properties are simple to formulate; however, the results are somewhat surprising and depend in an important way on the global nature of the full first-passage path. In the “ballistic limit”, where $X^2 \gg DT$, the space-time trajectory of the first-passage path approaches a straight line. In this case, intermediate-crossing properties are close to those that arise by treating the first-passage trajectory as purely ballistic. In the opposite “diffusive limit”, where $X^2 \ll DT$, the first-passage path is typically repelled from its final location X so as to avoid hitting X before time T .

Correspondingly, the probability distribution of times for the particle to first cross an intermediate level $0 < x < X$ undergoes a transition from unimodality, for $X^2 \gg DT$, to bimodality, for $X^2 \ll DT$. In the latter case, the first-passage path to (X, T) is most likely to cross an intermediate level near the beginning or near the end of its trajectory. In this bimodal regime, the distribution of the first-crossing times is reminiscent of, but more singular than, the famous arcsine law [3,4] for the distribution of times that a one-dimension Brownian particle spends on one side of the origin, as well as the distribution of the last passage time at the origin.

As a preliminary, we first investigate intermediate crossing phenomena for a purely Brownian path between $(0, 0)$ and (X, T) in section 2. In spite of the simplicity of this problem, the distributions of the first- and last-crossing times of an intermediate $0 < x < X$ level are also quite rich and have a qualitatively similar unimodal to bimodal transition as in the case where the trajectory is a first-passage path. Moreover, the boundary in phase space that demarcates this transition is, surprisingly, not single valued. In section 3, we investigate intermediate crossing properties when the trajectory between $(0, 0)$ and (X, T) is a first-passage path. We briefly discuss the situation where the intermediate level is negative in section 4. Finally, we offer some perspectives in section 5.

2. Preliminaries: Intermediate Crossings for Unconstrained Brownian Motion

Consider a Brownian particle in one dimension that starts at the origin. We will make extensive use of two important characteristics of this Brownian motion: (i) the occupation probability and (ii) the first-passage probability. These quantities are, respectively:

$$P(X, T) = \frac{1}{\sqrt{4\pi DT}} e^{-X^2/4DT} \quad F(X, T) = \frac{|X|}{\sqrt{4\pi DT^3}} e^{-X^2/4DT}. \quad (1)$$

Here $P(X, T)$ is the probability that a Brownian particle moves a distance X from its starting point over a time T , while $F(X, T)$ is the probability that the particle *first* reaches this point at time T [29]. One of the intriguing aspect of a Brownian trajectory

in one dimension is that it ultimately reaches any point on the infinite line. However, even though the trajectory is guaranteed to eventually reach any point $X \neq 0$, the mean time to reach an arbitrary point is infinite. This dichotomy arises because the probability that the trajectory first reaches position X at time T asymptotically decays as $T^{-3/2}$, from which the mean time to reach X is infinite.

For a Brownian particle that starts at $(0, 0)$ and ends at (X, T) , we now ask: where is the particle and what is its probability distribution of positions at an earlier time $t < T$? The probability that the particle propagates from $(0, 0)$ to (X, T) may be written as the convolution of the probabilities for the path from $(0, 0)$ to (x, t) and the path from (x, t) to the final location (X, T) :

$$\begin{aligned} P(X, T) &= \int P(x, t) P(X-x, T-t) dx \\ &= \int \frac{e^{-x^2/4Dt}}{\sqrt{4\pi Dt}} \frac{e^{-(X-x)^2/4D(T-t)}}{\sqrt{4\pi D(T-t)}} dx. \end{aligned} \quad (2)$$

Integrating over x reproduces, after some simple algebra, $P(X, t)$ in Eq. (1). For later convenience we introduce the dimensionless time $\tau = t/T$ and the dimensionless length $\chi = x/X$. By maximizing the integrand with respect to x , it is straightforward to derive that the integrand has its maximum when $x = \tau X$. That is, the particle moves a fraction τ of the final distance in a fraction τ of the total time, a well-known property of Brownian motion [28].

Finally, we compute the probability $\mathcal{P}(x, t)$ that the particle is at x at time t , given that it is at X at time T . This quantity equals the probability for the subset of Brownian paths from $(0, 0)$ to (X, T) that reach x at time t divided by the probability for all Brownian paths from $(0, 0)$ to (X, T) :

$$\begin{aligned} \mathcal{P}(x, t) &= \frac{P(x, t) P(X-x, T-t)}{P(X, T)} \\ &= \frac{e^{-x^2/4Dt}}{\sqrt{4\pi Dt}} \frac{e^{-(X-x)^2/4D(T-t)}}{\sqrt{4\pi D(T-t)}} \times \sqrt{4\pi DT} e^{X^2/4DT} \\ &= \frac{e^{-(x-\tau X)^2/4DT\tau(1-\tau)}}{\sqrt{4\pi DT\tau(1-\tau)}} \\ &\equiv \sqrt{\frac{\alpha}{\pi}} \frac{e^{-\alpha(\chi-\tau)^2/\tau(1-\tau)}}{\sqrt{\tau(1-\tau)}}, \end{aligned} \quad (3)$$

where we have rewritten the last line in terms of $\chi \in](-\infty, 1)$, $\tau \in (0, 1)$, and the dimensionless parameter $\alpha = X^2/4DT$, which demarcates whether the full trajectory is ballistic, for $\alpha \gg 1$, or diffusive, for $\alpha \ll 1$.

From Eq. (3), the probability distribution to reach an intermediate point x at dimensionless time τ is a Gaussian centered at $\chi = \tau$ whose width $\sqrt{\tau(1-\tau)}$ is maximal for $\tau = \frac{1}{2}$ and vanishes for $\tau \rightarrow 0$ and $\tau \rightarrow 1$. The physical message from these results is that the average position of a Brownian particle that starts at $(0, 0)$ and ends at (X, T) interpolates linearly between 0 and X as the time increases from 0 to T [28].

In a similar vein, we now determine when the Brownian particle *first* crosses and *last* crosses an intermediate position $x < X$, given that the particle is at X (not necessarily for the first time) at time T . More generally, we compute the probability distributions for these two events. Using the same reasoning that led to Eq. (3), the probability $\mathcal{F}(x, t)$ that the particle *first crosses* x at time t is given by:

$$\mathcal{F}(x, t) = \frac{F(x, t) P(X - x, T - t)}{P(X, T)}. \quad (4a)$$

That is, the first-crossing probability equals the probability for a Brownian particle, which starts at $(0, 0)$, to *first* reach (x, t) —hence the factor $F(x, t)$ —times the probability that the particle propagates from (x, t) to (X, T) , normalized by the probability for all Brownian paths that propagate from $(0, 0)$ to (X, T) .

Similarly, the probability $\mathcal{L}(x, t)$ that the *last crossing* of x occurs at time t is:

$$\mathcal{L}(x, t) = \frac{P(x, t) F(X - x, T - t)}{P(X, T)}. \quad (4b)$$

The reasoning that underlies (4b) is slightly more involved than that for (4a). For (x, t) to be the last crossing, the remaining trajectory must be a time-reversed first-passage path from (X, T) to (x, t) . This constraint guarantees that the crossing at x is the last one in the full trajectory to (X, T) .

Substituting the explicit forms for the occupation and first-passage probabilities from Eqs. (1) and performing some straightforward algebra, the first-crossing and last-crossing probabilities are, after expressing all variables in dimensionless form:

$$\begin{aligned} \mathcal{F}(\chi, \tau) &= \sqrt{\frac{\alpha}{\pi}} \frac{|\chi|}{\sqrt{\tau^3(1-\tau)}} e^{-\alpha(\chi-\tau)^2/[\tau(1-\tau)]}, \\ \mathcal{L}(\chi, \tau) &= \sqrt{\frac{\alpha}{\pi}} \frac{|1-\chi|}{\sqrt{\tau(1-\tau)^3}} e^{-\alpha(\chi-\tau)^2/[\tau(1-\tau)]}. \end{aligned} \quad (5)$$

It is apparent that $\mathcal{F}(\chi, \tau) = \mathcal{L}(1-\chi, 1-\tau)$, and vice versa, so that we only need to study one of these quantities. Figure 2 shows the time dependence of the first-crossing probability $\mathcal{F}(\chi, \tau)$ for three representative values of α and χ . The first-crossing probability clearly becomes bimodal for small α and $\chi \rightarrow 1$. On the other hand, for $\alpha \rightarrow \infty$, so that the trajectory becomes progressively more ballistic, the first- and last-crossing probabilities must approach each other.

To determine where in the χ - α plane that the first-crossing probability changes from unimodal to bimodal, we first need to locate the extrema of $\mathcal{F}(\chi, \tau)$ for each value of χ . Differentiating $\mathcal{F}(\chi, \tau)$ with respect to τ and setting the result to zero gives the cubic equation

$$4\tau^3 + (2\alpha - 4\alpha\chi - 7)\tau^2 + (3 + 4\alpha\chi^2)\tau - 2\alpha\chi^2 = 0, \quad (6a)$$

and solving for α gives

$$\alpha = \frac{(4\tau^3 - 7\tau^2 + 3\tau)}{[(4\chi - 2)\tau^2 - 4\chi^2\tau + 2\chi^2]}. \quad (6b)$$

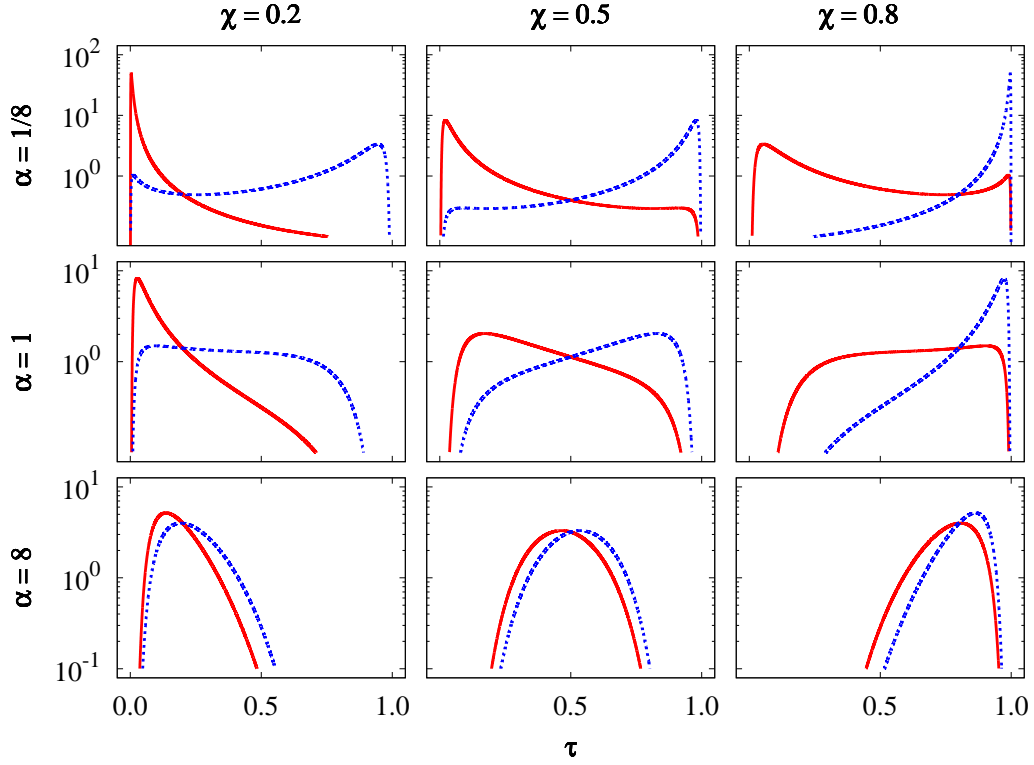


Figure 2. First-crossing probability $\mathcal{F}(\chi, \tau)$ (red, solid) and last-crossing probability $\mathcal{L}(\chi, \tau)$ (blue, dashed) for illustrative values of $\alpha = X^2/4DT$ and $\chi = x/X$ when the initial trajectory is an otherwise unrestricted Brownian path from $(0, 0)$ to (X, T) . For small α , $\mathcal{F}(\chi, \tau)$ changes from unimodal to bimodal as χ increases. For large α (almost ballistic trajectory), the first-crossing and last-crossing times are close to each other.

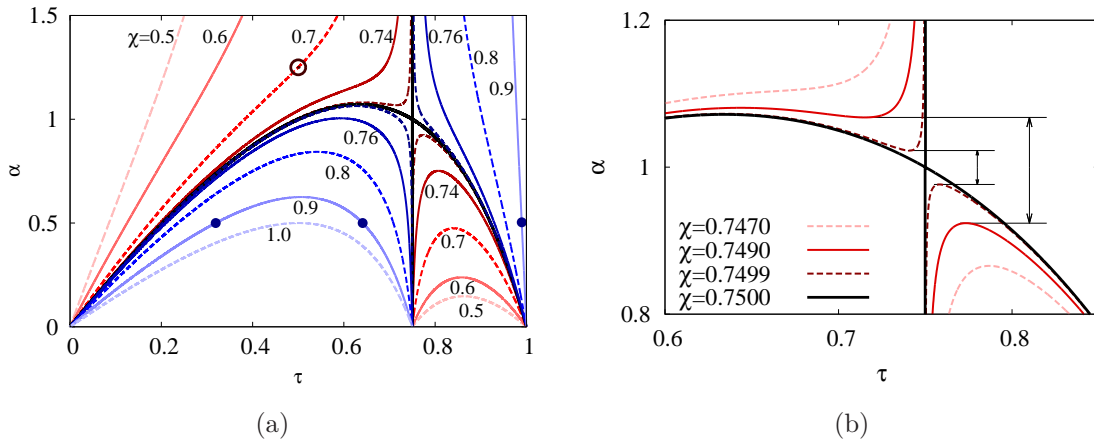


Figure 3. (a) Loci of the extrema of $\mathcal{F}(\chi, \tau)$ in the α - τ plane for various values of χ when the initial trajectory is an otherwise unrestricted Brownian path to (X, T) . For a given α and χ , the extrema occur at the values of τ where the line $\alpha = \text{const.}$ intersects the curve that corresponds to a given χ . (b) Zoom near the critical point $(\frac{3}{4}, 1)$

These loci for α are plotted as a function of τ for various values of χ in Fig. 3(a). For given α and χ , the extrema occur at the τ values where the line $\alpha = \text{const.}$ intersects the branches of the curve for a given χ . For example, in Fig. 3(a), when $\alpha = 0.5$ and $\chi = 0.9$, \mathcal{F} has three extrema at $\tau = 0.32, 0.64$, and 0.99 (two maxima and an intermediate minimum), as indicated by the dots. On the other hand for $\alpha = 1.25$ and $\chi = 0.7$, there is a single extremum (circle). When $\chi \approx 0.75$, the regime of bimodality extends over the widest range of α . We plot the phase boundary (Fig. 4) on the χ - α plane by scanning across χ and numerically finding the range of α values at which three extrema occur.

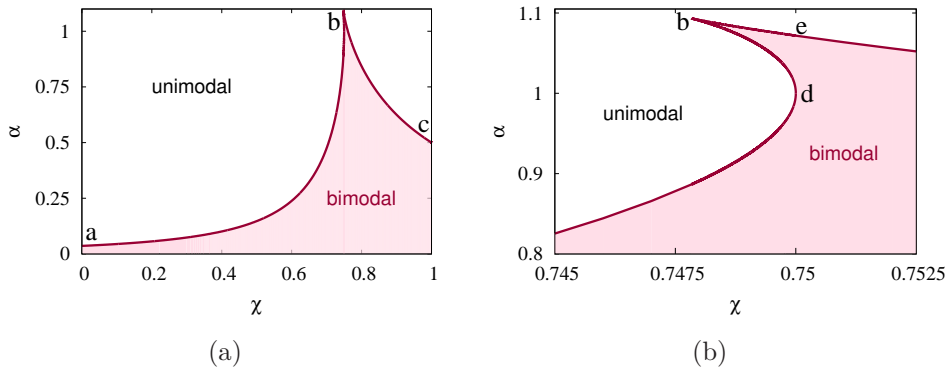


Figure 4. (a) Numerically obtained phase diagram from Eq. (6), showing the domains in the parameter space where the first-crossing probability is unimodal and where it is bimodal for an unrestricted Brownian path from $(0,0)$ to (X,T) . The points marked a, b, c are at $(0, \frac{7}{2} - 2\sqrt{3})$, $(0.747835 \dots, 1.09325 \dots)$, and $(1, \frac{1}{2})$, respectively. (b) Detail near the cusp in the phase boundary; the points marked d, e are at $(\frac{3}{4}, 1)$ and $(\frac{3}{4}, 4(2 - \sqrt{3}))$, respectively.

The behavior near the critical point $(\tau, \alpha) = (\frac{3}{4}, 1)$ is particularly intriguing (Fig. 3(b)). For a given value of χ that is less than but very close to $\chi = 3/4$, there are two distinct sets of solutions—one set with α slightly less than 1 and another set with α slightly larger than 1. There is also a small gap between these two solution sets, as indicated in Fig. 3(b) for the cases $\chi = 0.749$ and $\chi = 0.7499$. The consequence of this feature is that the unimodal to bimodal phase boundary is not single valued near the cusp, as shown in Fig. 4. It is quite remarkable that such a simple question about a Brownian path—namely the time for the path to cross an intermediate position—leads to such a rich phenomenon.

3. Intermediate Crossings for First-Passage Paths

We now turn to the properties of intermediate crossings for first-passage paths, where the first-passage constraint for the full trajectory from $(0,0)$ to (X,T) significantly affects the global nature of intermediate trajectory and concomitantly, the intermediate crossings. We divide our discussion into: (i) the location of the particle at an arbitrary

intermediate time and (ii) the time when the particle crosses an arbitrary intermediate position.

3.1. Intermediate Crossing Position

At a time $t < T$, we again ask: what is the probability $\mathcal{P}(x, t)$ that the particle is at position x , given that the particle first reaches X at time T ? We determine this probability, following the same approach that led to Eq. (3), by decomposing the trajectory into the segment up to time t and the remaining segment from $T - t$ to T . The first segment is a Brownian path to (x, t) , but now subject to the constraint that it can not reach X , because reaching X would mean that the full trajectory is not a first-passage path to (X, T) . To implement this constraint we impose an absorbing boundary condition at X by augmenting the initial Gaussian with an anti-Gaussian image distribution that is centered at $2X$ [3, 29]. We denote the probability distribution in the presence of this absorbing boundary condition as $P_A(x, t)$. The second segment from $T - t$ to time T is simply a first-passage path between these two points.

Assembling these elements, we have

$$\begin{aligned} \mathcal{P}(x, t) &= \frac{P_A(x, t) F(X - x, T - t)}{F(X, T)} \\ &= \frac{\frac{1}{\sqrt{4\pi Dt}} \left[e^{-x^2/4Dt} - e^{-(2X-x)^2/4Dt} \right] \frac{|X-x|}{\sqrt{4\pi D(T-t)^3}} e^{-(X-x)^2/4D(T-t)}}{\frac{|X|}{\sqrt{4\pi DT^3}} e^{-X^2/4DT}}. \end{aligned} \quad (7)$$

By expressing all quantities in terms of the dimensionless variables introduced previously, the above expression simplifies to

$$\begin{aligned} \mathcal{P}(\chi, \tau) &= \sqrt{\frac{\alpha}{\pi}} \frac{|1-\chi|}{\sqrt{\tau(1-\tau)^3}} e^{-\alpha[(1-\chi)^2 - (1-\tau)]/(1-\tau)} \left[e^{-\alpha\chi^2/\tau} - e^{-\alpha(2-\chi)^2/\tau} \right] \\ &= \sqrt{\frac{\alpha}{\pi}} \frac{|1-\chi|}{\sqrt{\tau(1-\tau)^3}} e^{-\alpha(\chi-\tau)^2/[\tau(1-\tau)]} \left[1 - e^{-4\alpha(1-\chi)/\tau} \right]. \end{aligned} \quad (8)$$

Notice that τ lies in $(0, 1)$ by construction, but χ can range from $-\infty$ to 1.

The behavior of $\mathcal{P}(\chi, \tau)$ is quite rich, as illustrated in Fig. 5. For small α (diffusive limit), the particle must initially move in the negative- x direction so as to ensure that it does not hit X before time T . A related type of repulsion arises in the positions of a set of N random walkers that all start a finite distance away from an absorbing point subject to the constraint that none of them are absorbed up to a given time [30]. As α is increased, corresponding to a more ballistic and hence more deterministic trajectory from $(0, 0)$ to (X, T) , the spread in the probability distribution correspondingly decreases.

The extent of the repulsion may be quantified by the minimum value of $x_{\text{mp}}(\tau)$, the most probable location of the trajectory as a function of rescaled time. For $\alpha \rightarrow 0$, the difference between the initial and final positions becomes immaterial so that we can

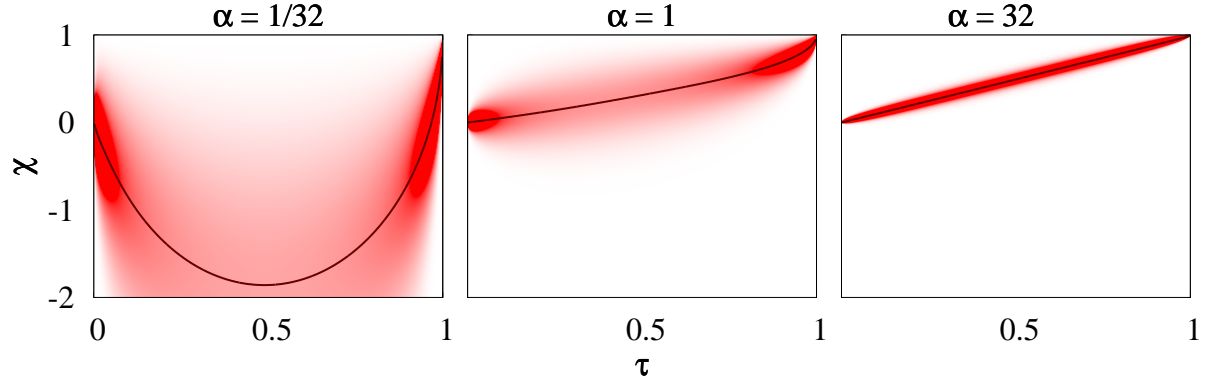


Figure 5. Heatmaps of the conditional occupation probability $\mathcal{P}(\chi, \tau)$ for a first-passage path from $(0,0)$ to (X,T) for illustrative values of α in the τ - χ plane. The smooth curve shows the time dependence of the most probable location of the particle. For small α , the trajectory is initially repelled from its final destination. The distribution is most diffuse near $\tau = \frac{1}{2}$ and most localized near $\tau = 0$ and $\tau = 1$.

approximate the minimum value of $x_{\text{mp}}(\tau)$ by $x_{\text{mp}}(\tau = \frac{1}{2})$. Using this simplification in Eq. (8), the probability distribution at $\tau = \frac{1}{2}$ reduces to

$$\mathcal{P}(y, \frac{1}{2}) \propto \sqrt{\alpha} e^{-\alpha} y e^{-4\alpha y^2} \sinh(4\alpha y), \quad (9)$$

where $y = \chi - 1$. Finding the maximum of this latter expression is now elementary and we find that for $\alpha \rightarrow 0$, the minimum on the most probable trajectory is located at

$$y^* \simeq -\frac{1}{2\sqrt{\alpha}}. \quad (10)$$

Thus for $\alpha \rightarrow 0$, the most probable trajectory is strongly repelled from the final point for $\tau < 1/2$ and subsequently is strongly attracted to this final point. We note that this behavior for y^* can also be inferred from a macroscopic fluctuation theory, as given in Ref. [30].

3.2. Intermediate Crossing Times

Parallel to the discussion given for the pure Brownian path, we now compute the distribution of times when the first-passage trajectory to (X,T) crosses an intermediate level $x \in (0, X)$. We shall consider the case $x < 0$ separately in section 4 as the calculation details are different. We also separately consider the cases of the first crossing and the last crossing because the calculational details and the results for these two cases are quite different.

3.2.1. First-crossing probability As in the case where the full trajectory is an unconstrained Brownian path that starts at $(0,0)$ and ends at (X,T) , we decompose the trajectory into an initial segment that starts at $(0,0)$ and crosses x for the first time

at time t , and a final segment that starts at (x, t) and crosses X for the first time at time T . We consider here the case $x > 0$; the case $x < 0$ will be treated in the next section. Here the analog of Eq. (4a) is

$$\mathcal{F}(x, t) = \frac{F(x, t) F(X - x, T - t)}{F(X, T)}. \quad (11)$$

We now substitute the relevant first-passage probabilities from (1) into the above equation to obtain

$$\mathcal{F}(x, t) = \frac{|x|}{\sqrt{4\pi Dt^3}} e^{-x^2/4Dt} \frac{|X - x|}{\sqrt{4\pi D(T - t)^3}} e^{-(X - x)^2/4D(T - t)} \bigg/ \frac{|X|}{\sqrt{4\pi DT^3}} e^{-X^2/4DT}. \quad (12)$$

In terms of the dimensionless variables α , χ , and τ , the above expression simplifies, after some straightforward algebra, to

$$\mathcal{F}(\chi, \tau) = \sqrt{\frac{\alpha}{\pi}} \frac{|1 - \chi| |\chi|}{[(1 - \tau)\tau]^{3/2}} e^{-\alpha(\tau - \chi)^2/[\tau(1 - \tau)]}. \quad (13)$$

Once again, the qualitative behavior of this first-crossing probability depends in an essential way on the value of α (Fig. 6). For large α (ballistic limit) $\mathcal{F}(\chi, \tau)$ is sharply peaked about the point $\tau = \chi$. Thus in this ballistic limit, the most probable time for a Brownian particle to first reach a distance x is simply equal to x . Moreover, the distribution in (13) reduces to a Gaussian form for $\tau \approx \chi$.

Conversely, in the diffusive limit of $\alpha \rightarrow 0$, and for $\tau \gg \alpha$ and $1 - \tau \gg \alpha$ (i.e., τ not too close to 0 or 1), the probability density function is controlled by the factor $[\tau(1 - \tau)]^{-3/2}$, which is similar to, but more singular than the arcsine law [4]. The surprising result for this limit is that a Brownian particle is most likely to cross an arbitrary intermediate level either at the very beginning or at the very end of its trajectory.

A remarkable aspect of the first-crossing probability (13) is its invariance under the simultaneous interchanges $\tau \rightarrow 1 - \tau$ and $\chi \rightarrow 1 - \chi$. We can give a simple graphical argument to justify this symmetry (Fig. 7). In (a), a first-passage path from $(0, 0)$ to (X, T) is comprised of a first crossing (dashed) to (χ, τ) (in scaled units) and the remaining segment to (X, T) (solid). Interchanging these two segments leads to a first-crossing segment to $(1 - \chi, 1 - \tau)$ and the remaining segment to (X, T) . Since the segments are independent, the probability for these two first-passage paths in the figure are identical and thus $\mathcal{F}(\chi, \tau) = \mathcal{F}(1 - \chi, 1 - \tau)$.

We can apply this same perspective to argue that \mathcal{F} is bimodal for $\alpha \ll 1$. Indeed, let us compare a first-passage path to the final point that has its first crossing close to $\tau = 0$ or $\tau = 1$, and a first-passage path that has its first crossing near $\tau = 1/2$. In the former case (see Fig. 8(a)), the remainder of the path away from the first crossing must be repelled from the final point. The probability for such a first-passage path from $(0, 0)$

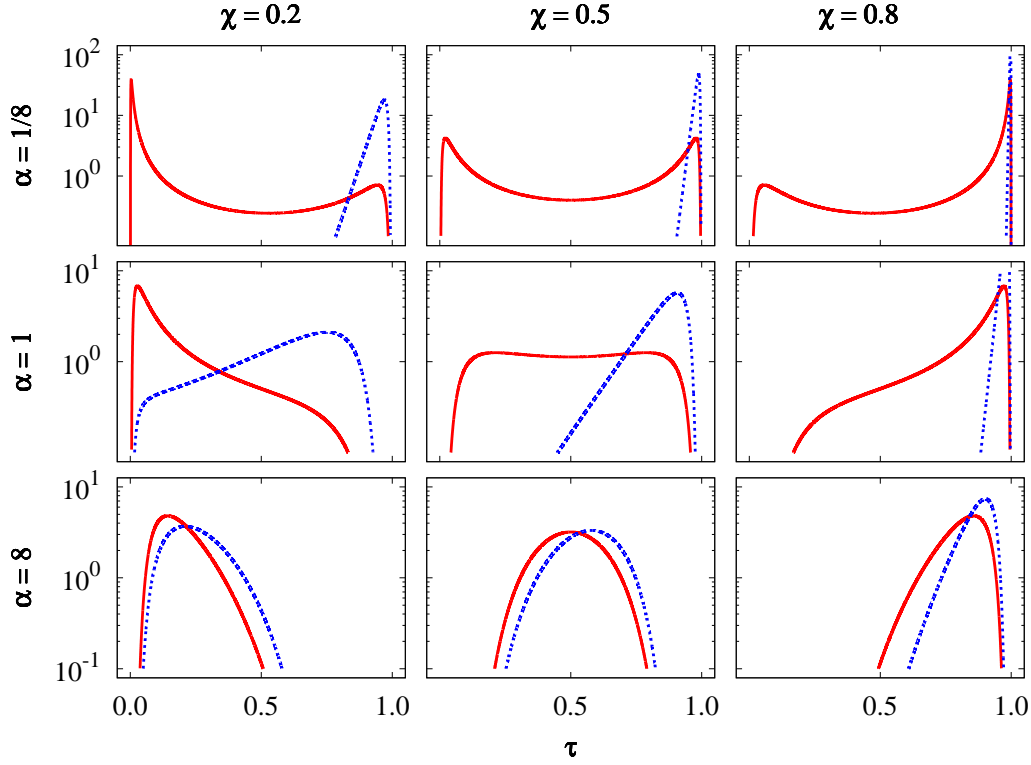


Figure 6. First-crossing probability $\mathcal{F}(\chi, \tau)$ (red, solid) and the last-crossing probability $\mathcal{L}(\chi, \tau)$ (blue, dashed) for illustrative values of α and χ when the initial trajectory is a first-passage path from $(0, 0)$ to (X, T) . For small α , $\mathcal{F}(\chi, \tau)$ is bimodal while $\mathcal{L}(\chi, \tau)$ is unimodal and sharply peaked as $\tau \rightarrow 1$. For large α (almost ballistic trajectory), the first-crossing and last-crossing times nearly coincide.

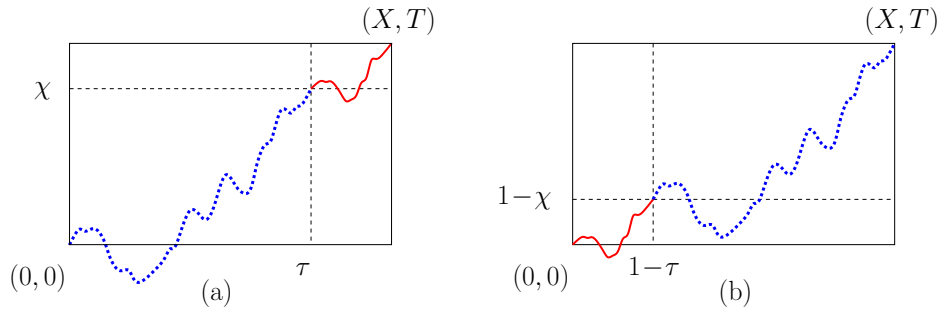


Figure 7. (a) A first-passage path that consists of a solid and dashed segment with a first-crossing at (χ, τ) . Interchanging the order of these segments gives a first-crossing at $(1-\chi, 1-\tau)$.

to (X, T) scales as $T^{-3/2}$ for $\alpha \ll 1$. On the other hand, the probability for a path that first-crosses χ near $T/2$ is the product of the probabilities of two first-passage paths of duration $T/2$, namely $(T^{-3/2}/2)^2$, which is much less than $T^{-3/2}$. Thus a first-crossing near $T/2$ is unlikely for $\alpha \ll 1$.

To determine where in the phase space the transition in \mathcal{F} between unimodality and

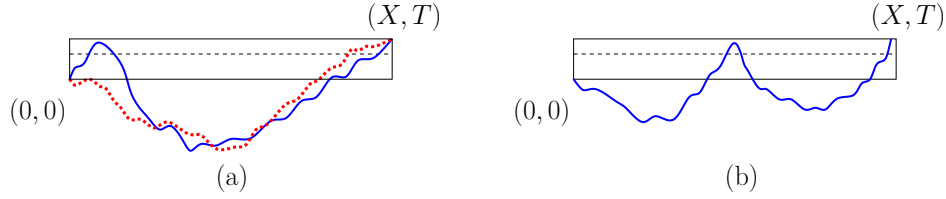


Figure 8. (a) First-passage paths that first cross an intermediate level near $\tau = 0$ or $\tau = 1$ on an exaggerated scale to emphasize the limit $\alpha \ll 1$. (b) A first-passage path that first crosses the intermediate level near $\tau = \frac{1}{2}$.

bimodality occurs, we again determine the extrema of \mathcal{F} . Following the same procedure that led to Eq. (6), we obtain the cubic equation for the location of the extrema

$$6\tau^3 + (2\alpha - 4\alpha\chi - 9)\tau^2 + (3 + 4\alpha\chi^2)\tau - 2\alpha\chi^2 = 0, \quad (14)$$

and the resulting solutions for α are plotted as a function of τ for various values of χ in Fig. 9(a). For given α and χ , the extrema occur at the τ values where the line $\alpha = \text{const.}$ intersects the curve corresponding to a given χ . Figure 9(b) shows the region of the phase diagram where the first-crossing probability is unimodal and where it is bimodal. Here the phase boundary is everywhere single valued, in contrast to the case of Fig. 4 the initial path is an unrestricted Brownian motion. As a result of the symmetry of \mathcal{F} , the phase diagram is symmetric about the point $\chi = \frac{1}{2}$. Also, unlike in the case of unconstrained Brownian path, the phase boundary is single-valued.

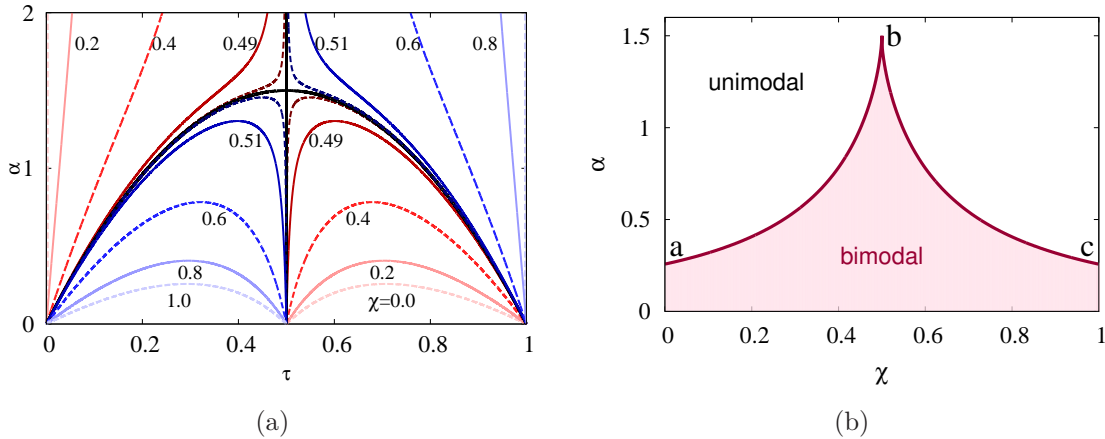


Figure 9. (a) Loci of the extrema of $\mathcal{F}(\chi, \tau)$ in the α - τ plane for various values of χ when the initial trajectory is a first-passage path to (X, T) . For a given α and χ , the extrema occur at the values of τ where the line $\alpha = \text{const.}$ intersects the curve that corresponds to a given χ . (b) Numerically obtained phase diagram from Eq. (14), showing where in the parameter space the first-crossing probability, for a first-passage Brownian path from $(0, 0)$ to (X, T) , is unimodal and where it is bimodal. The points marked a, b, c are at $(0, \frac{9}{2} - 3\sqrt{2})$, $(\frac{1}{2}, \frac{3}{2})$, and $(1, \frac{9}{2} - 3\sqrt{2})$, respectively.

3.2.2. Last-crossing probability We now determine when the particle crosses a specified intermediate level for the *last* time. In principle, we may perform this calculation by decomposing the trajectory into an initial segment from $(0,0)$ to the last crossing of x at time t , and a remaining first-passage segment from (x,t) to (X,T) . The subtle feature here is that this second segment must also obey the constraint that this segment always remains greater than x , so that no additional crossings of x occur after time t . To satisfy the latter condition, we must also impose an absorbing boundary condition at x . Thus the particle begins the second segment at the absorbing boundary, so that the first-passage probability to (X,T) would equal zero. To sidestep this pathology, we could start the particle at $x+dx$ and take the limit dx at the end of the calculation. This limiting process is a delicate, however, and we therefore give an alternative approach that avoids any limiting processes. The price, however, is the necessity to break the trajectory into three segments (Fig. 10).

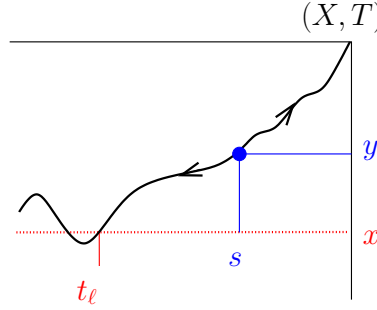


Figure 10. Zoom of the first-passage path in Fig. 1, with the decomposition of the segment from t_ℓ to T into a time-reversed first-passage path from (y, s) to (x, t_ℓ) and a first-passage path from (y, s) to (X, T) .

In this alternative approach, the first segment is a Brownian path that starts at $(0,0)$ and reaches the last crossing of x at time t_ℓ . An absorbing boundary at X must be imposed to ensure that this segment never reaches X before T . We now break the remaining segment from (x, t_ℓ) to (X, T) , into two sub-segments with respect to an arbitrary point (y, s) , with $x < Y < X$ and $t_\ell < s < T$. The left sub-segment is a backward-propagating first-passage path from (y, s) to (x, t_ℓ) and the right sub-segment is a forward-propagating first-passage path from (y, s) to (X, T) . The choice of intermediate point (y, s) is arbitrary, so that the final result must be independent of s after integrating over all y .

Thus we have

$$\mathcal{L}(x, t) = \frac{P_A(x, t) \int_x^X F_A(y - x, s - t) F_A(X - y, T - s) dy}{F(X, T)}. \quad (15)$$

Here $F_A(z, t)$ denotes the first-passage probability in the presence of the absorbing boundary condition at X . Making use of standard results for the first-passage

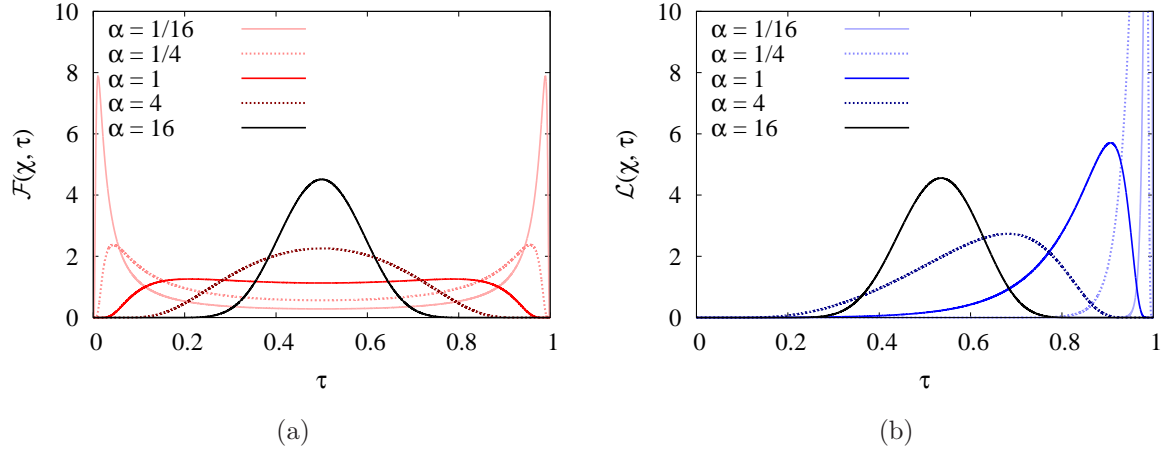


Figure 11. (a) Comparison of the first-crossing probability $\mathcal{F}(\chi, \tau)$ and (b) the last-crossing probability $\mathcal{L}(\chi, \tau)$ for representative values of α for the specific case of $\chi = 1/2$. As α increases $\mathcal{F}(\chi, \tau)$ remains symmetric, but changes from bimodal to unimodal, while $\mathcal{L}(\chi, \tau)$ merely moves systematically toward $\tau = 1$.

probability in the interval [29], the integral in (15) is

$$\begin{aligned}
 & \int_x^X F_A(y-x, s-t) F_A(X-y, T-s) dy \\
 &= \int_x^X \frac{4\pi^2 D^2}{(X-x)^4} \sum_{m,n=1}^{\infty} (-1)^m n m \sin\left(\frac{n\pi y}{X-x}\right) \sin\left(\frac{m\pi y}{X-x}\right) e^{-\pi^2 D[n^2(s-t)+m^2(T-s)]/(X-x)^2} dy \\
 &= \frac{2\pi^2 D^2}{(X-x)^3} \sum_{n=1}^{\infty} (-1)^n n^2 e^{-n^2 \pi^2 D(T-t)/(X-x)^2}.
 \end{aligned} \tag{16}$$

To obtain the third line, the orthogonality relation $\int_0^1 2 \sin(n\pi x) \sin(m\pi x) dx = \delta_{mn}$ has been used.

Substituting the above expression, together with the previously derived forms for $P_A(x, t)$ and $F(X, T)$ in Eq. (15), and using the dimensionless variables χ , τ and α , we finally obtain

$$\mathcal{L}(x, t) = \left(\frac{\pi^2 e^\alpha}{8\alpha^2 \sqrt{\tau} (1-\chi)^3} \right) \left[e^{-\alpha\chi^2/\tau} - e^{-\alpha(2-\chi)^2/\tau} \right] \left[\sum (-1)^n n^2 e^{-n^2 \pi^2 (1-\tau)/[4\alpha(1-\chi)^2]} \right]. \tag{17}$$

When $\alpha \ll 1$, for $1-\tau \gg \alpha$ (τ not too close to 1), the first term in the sum dominates and the last-crossing probability reduces to

$$\mathcal{L}(\chi, \tau) \sim \frac{e^{-A(1-\tau)}}{\tau^{1/2}}, \tag{18}$$

with $A = \pi^2/[4\alpha(1-\chi)^2]$. In this limit, the last-crossing probability increases exponentially with τ as $\tau \rightarrow 1$ (Fig. 11). Conversely, when $\alpha \gg 1$, the last-crossing probability is sharply peaked at $\tau = \chi$. This feature is a result of the trajectory becoming nearly ballistic. When $\alpha \gg 1$, the first and last crossing times coincide because there is little stochasticity in the trajectory.

4. First and Last Crossings to $x < 0$

Thus far, we have tacitly assumed that the intermediate position is between 0 and X . With this constraint, every path from $(0,0)$ to (X,T) must necessarily pass through any intermediate position. We now investigate the first- and last-crossing probabilities when the intermediate position $x < 0$. Here the probability that a first-passage path from $(0,0)$ to (X,T) actually reaches x is less than one. The decomposition of the first passage path into a segment from the start to the crossing point and from the crossing point to the final point still applies, but there are additional subtleties associated with the intermediate point being negative.

Again, we separately consider the first- and last-crossing probabilities. It is convenient to define $z = |x|$, which is manifestly positive. The distribution of first-crossing times to z is formally given by

$$\mathcal{F}(z, t) = \frac{F_A(z, t) F(X + z, T - t)}{F(X, T)}. \quad (19)$$

The constituent first-passage probability $F_A(z, t)$ is subject to the constraint that X cannot be reached before time t ; this requirement ensures that the full path is actually a first-passage trajectory to (X, T) . The second segment from (z, t) to (X, T) is a first-passage path between these two points without any additional constraints.

To obtain $F_A(z, t)$, we again solve the diffusion equation in the interval between $z = -x$ and X , with absorbing boundary conditions at both ends, and then compute the flux to the boundary point z for a particle that starts at the origin. By standard methods [29], this computation gives

$$F_A(z, t) = \frac{2\pi D}{(X + z)^2} \sum_{n=1}^{\infty} n \sin\left(\frac{n\pi z}{X + z}\right) e^{-n^2\pi^2 Dt/(X+z)^2}. \quad (20)$$

Thus the first-crossing probability is

$$\mathcal{F}(z, t) = \frac{\frac{2\pi D}{(X+z)^2} \sum_{n=1}^{\infty} n \sin\left(\frac{n\pi z}{X+z}\right) e^{-n^2\pi^2 Dt/(X+z)^2} \frac{|X+z|}{\sqrt{4\pi D(T-t)^3}} e^{-(X+z)^2/4D(T-t)}}{\frac{|X|}{\sqrt{4\pi DT^3}} e^{-X^2/4DT}} \quad (21)$$

In dimensionless variables, the above expression simplifies to

$$\mathcal{F}(\chi, \tau) = \frac{\pi e^{\alpha[1-\tau-(1+\chi)^2]/(1-\tau)}}{2\alpha(1+\chi)(1-\tau)^{3/2}} \sum_{n=1}^{\infty} n \sin\left(\frac{n\pi\chi}{1+\chi}\right) e^{-n^2\pi^2\tau/[4\alpha(1+\chi)^2]}. \quad (22)$$

For $\alpha \rightarrow 0$, for $\tau \gg \alpha$, the first term in the sum is dominant so that

$$\mathcal{F}(\chi, \tau) \sim \frac{e^{-A\tau}}{(1-\tau)^{3/2}} \quad \alpha \rightarrow 0, \quad (23)$$

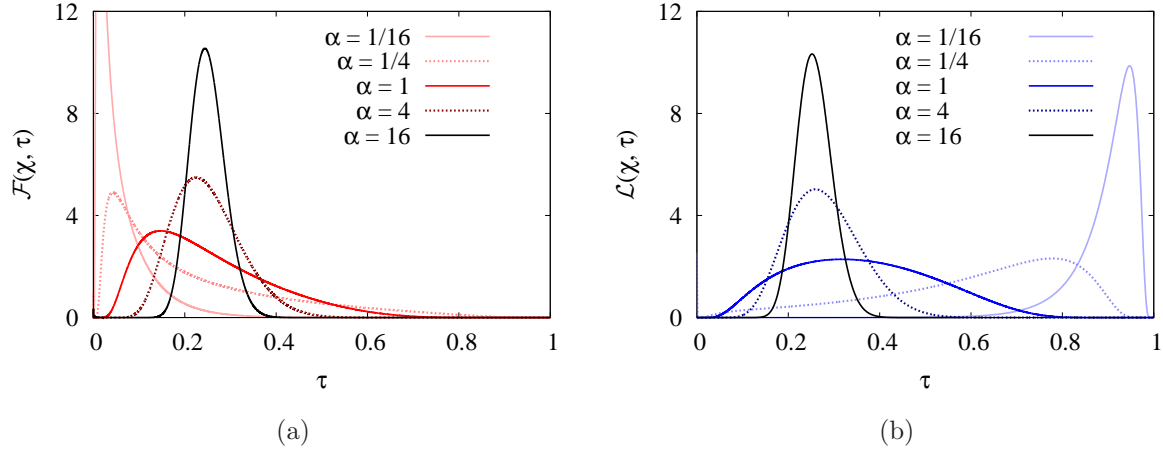


Figure 12. (a) The first-crossing probability $\mathcal{F}(\chi, \tau)$ and (b) the last-crossing probability $\mathcal{L}(\chi, \tau)$ for $\chi = -1/2$ for a range of α values. The distributions have been rescaled so that they fit on the same range.

with $A = \pi^2/[4\alpha(1+\chi)^2]$. Conversely, for $\alpha \rightarrow \infty$, Fig. 12 shows that $\mathcal{F}(\chi, \tau)$ is peaked at $\tau = \frac{\chi}{1+\chi}$. The particle thus moves ballistically in the negative- x direction to reach $-x$ in a fraction $\frac{\chi}{1+\chi}$ of the total time and then moves ballistically in the positive- x direction to reach X at time T .

The distribution of last-crossing times has the identical form to that given in Eq. (17) for the case where $x > 0$, except for the substitution $x \rightarrow -x$. For $\alpha \ll 1$, the last crossing necessarily occurs very close to the final time $\tau = 1$. For $\alpha \gg 1$, the overall trajectory is a straight line in the negative- x direction to the intermediate point and then another straight line in the positive- x direction to the final point. In this limit, the first- and last-crossing probabilities become progressively more similar, as expected intuitively.

5. Summary and Outlook

We investigated the properties of intermediate crossings of Brownian and first-passage paths in one dimension that start at $(0, 0)$ and end at a final point (X, T) . By using simple probabilistic arguments, we analytically determined the occupation probability at a general intermediate time, as well as the first-crossing and last-crossing times at a general intermediate location. These intermediate properties exhibit a number of surprising and anomalous features that depend, in an essential way, on $\alpha = X^2/4DT$. In the ballistic limit of $\alpha \gg 1$, a trajectory typically moves systematically from the starting point to the final point. In this case, one can infer intermediate-crossing properties by linearly interpolating the initial trajectory.

The more interesting situation of the diffusive limit, where $\alpha \ll 1$, a first-passage Brownian path to (X, T) must initially move away from this final point so as to not reach X before time T . The maximum excursion away from the starting point scales

as $1/\sqrt{\alpha}$. The behavior of the first-crossing probability, the distribution of times when a path first crosses a specified intermediate point x is quite rich. When the ostensibly simpler example where initial path is a Brownian trajectory to (X, T) with no additional constraint, the first-crossing probability can be either unimodal or bimodal, with bimodality favored for small α and $\chi = x/X \approx 0.75$. Moreover, the phase boundary between unimodality and bimodality is, quite surprisingly, not single valued. When the initial path is a first-passage path to (X, T) , the first-crossing probability again has a unimodal to bimodal transition and the corresponding phase diagram is symmetric in the α - χ plane.

Another unanticipated feature of the first- and last-crossing probabilities is that the results are invariant if there is an overall global drift in the Brownian trajectory. When one generalizes the expressions for the first- and last-crossing probabilities given in Eqs. (4), (11), and (15) to incorporate a constant drift, all factors that involve the drift velocity cancel out. It would be worthwhile to understand the full ramifications of this simple observation.

Finally, it is worth mentioning that the decomposition of the first-passage path in (11) provides the starting point for efficient simulations of intermediate crossing phenomena. The naive way to numerically determine intermediate crossing properties is by direct simulation of a random walk in which the times at which various intermediate positions are reached are recorded for a walk that reaches a given final point. From this data, one can reconstruct the first-crossing (as well as the last-crossing) probabilities. As a much more efficient alternative, one can first select a set of intermediate positions and then directly move a particle only between these intermediate positions. Correspondingly, the time between each of these macro-steps is incremented from the appropriate distribution of first passage times. This procedure can be made still more efficient by only allowing the walk to move to intermediate positions that are progressively closer to the final position. Thus arbitrarily long random walks can be simulated with a finite number of steps.

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